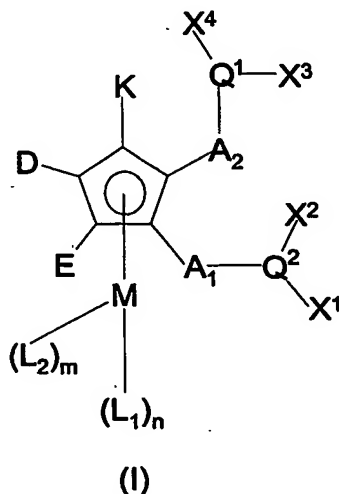


Claims

1. A compound obtainable by combining:
 - (a) a Group VIIIIB metal or a compound thereof; and,
 - 5 (b) a compound of formula I or salt thereof:



wherein:

- 10 A₁ and A₂, and A₃, A₄ and A₅ (when present), each independently represent lower alkylene;

K is selected from the group consisting of hydrogen, lower alkyl, aryl, Het, halo, cyano, nitro, -OR¹⁹, -OC(O)R²⁰,
 15 -C(O)R²¹, -C(O)OR²², -N(R²³)R²⁴, -C(O)N(R²⁵)R²⁶, -C(S)(R²⁷)R²⁸,
 -SR²⁹, -C(O)SR³⁰, -CF₃ or -A₃-Q³(X⁵)X⁶;

D is selected from the group consisting of hydrogen, lower alkyl, aryl, Het, halo, cyano, nitro, -OR¹⁹, -OC(O)R²⁰,
 20 -C(O)R²¹, -C(O)OR²², -N(R²³)R²⁴, -C(O)N(R²⁵)R²⁶, -C(S)(R²⁷)R²⁸,
 -SR²⁹, -C(O)SR³⁰, -CF₃ or -A₄-Q⁴(X⁷)X⁸;

E is selected from the group consisting of hydrogen, lower alkyl, aryl, Het, halo, cyano, nitro, -OR¹⁹, -OC(O)R²⁰,

$-C(O)R^{21}$, $-C(O)OR^{22}$, $-N(R^{23})R^{24}$, $-C(O)N(R^{25})R^{26}$, $-C(S)(R^{27})R^{28}$,
5 $-SR^{29}$, $-C(O)SR^{30}$, $-CF_3$ or $-A_5-Q^5(X^9)X^{10}$;

or both D and E together with the carbon atoms of the
5 cyclopentadienyl ring to which they are attached form an
optionally substituted phenyl ring:

X^1 represents $CR^1(R^2)(R^3)$, congressyl or adamantyl, X^2
represents $CR^4(R^5)(R^6)$, congressyl or adamantyl, or X^1 and
10 X^2 together with Q^2 to which they are attached form an
optionally substituted 2-phospha-adamantyl group, or X^1
and X^2 together with Q^2 to which they are attached form a
ring system of formula 1a;

15 X^3 represents $CR^7(R^8)(R^9)$, congressyl or adamantyl, X^4
represents $CR^{10}(R^{11})(R^{12})$, congressyl or adamantyl, or X^3
and X^4 together with Q^1 to which they are attached form an
optionally substituted 2-phospha-adamantyl group, or X^3
and X^4 together with Q^1 to which they are attached form a
20 ring system of formula 1b;

X^5 represents $CR^{13}(R^{14})(R^{15})$, congressyl or adamantyl, X^6
represents $CR^{16}(R^{17})(R^{18})$, congressyl or adamantyl, or X^5
and X^6 together with Q^3 to which they are attached form an
25 optionally substituted 2-phospha-adamantyl group, or X^5
and X^6 together with Q^3 to which they are attached form a
ring system of formula 1c;

X^7 represents $CR^{31}(R^{32})(R^{33})$, congressyl or adamantyl, X^8
30 represents $CR^{34}(R^{35})(R^{36})$, congressyl or adamantyl, or X^7
and X^8 together with Q^4 to which they are attached form an
optionally substituted 2-phospha-adamantyl group, or X^7

and X^8 together with Q^4 to which they are attached form a ring system of formula 1d;

X^9 represents $CR^{37}(R^{38})(R^{39})$, congressyl or adamantyl, X^{10}
5 represents $CR^{40}(R^{41})(R^{42})$, congressyl or adamantyl, or X^9
and X^{10} together with Q^5 to which they are attached form an
optionally substituted 2-phospha-adamantyl group, or X^9
and X^{10} together with Q^5 to which they are attached form a
ring system of formula 1e;

10

Q^1 and Q^2 , and Q^3 , Q^4 and Q^5 (when present), each
independently represent phosphorus, arsenic or antimony;

M represents a Group VIB or VIIIB metal or metal cation
15 thereof;

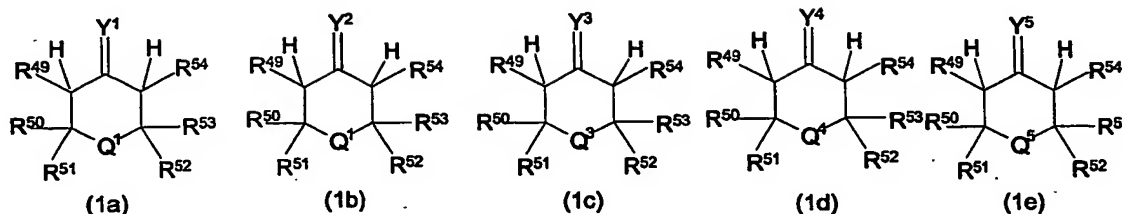
L_1 represents an optionally substituted cyclopentadienyl,
indenyl or aryl group;

20 L_2 represents one or more ligands each of which are
independently selected from hydrogen, lower alkyl,
alkylaryl, halo, CO, $P(R^{43})(R^{44})R^{45}$ or $N(R^{46})(R^{47})R^{48}$;

R^1 to R^{18} and R^{31} to R^{42} , when present, each independently
25 represent hydrogen, lower alkyl, aryl, halo or Het;

R^{19} to R^{30} and R^{43} to R^{48} , when present, each independently
represent hydrogen, lower alkyl, aryl or Het;

30 the ring systems of formula 1a, 1b, 1c, 1d and 1e are
represented by the formulae



R^{49} , R^{54} and R^{55} , each independently represent hydrogen, lower alkyl or aryl; R^{50} to R^{53} each independently represent hydrogen, lower alkyl, aryl or Het; and Y^1 , Y^2 , Y^3 , Y^4 and Y^5 , each independently represent oxygen, sulfur or N- R^{55} ;

$n = 0$ or 1 ;

and $m = 0$ to 5 ;

provided that when $n = 1$ then m equals 0 , and when n equals 0 then m does not equal 0 .

2. A compound as claimed in claim 1, wherein if both K represents $-A_3-Q^3(X^5)X^6$ and E represents $-A_5-Q^5(X^9)X^{10}$, then D represents $-A_4-Q^4(X^7)X^8$.

3. A compound as claimed in claim 1 or 2, wherein R^1 to R^{18} and R^{31} to R^{42} each independently represent hydrogen, optionally substituted C_1 - C_6 alkyl or optionally substituted phenyl.

4. A compound as claimed in any one of claims 1 to 3, wherein R^1 to R^{18} and R^{31} to R^{42} each independently represent hydrogen or non-substituted C_1 - C_6 alkyl.

5. A compound as claimed in any one of claims 1 to 3, wherein one or more of the groups R^1 to R^3 , R^4 to R^6 , R^7 to

R⁹, R¹⁰ to R¹², R¹³ to R¹⁵, R¹⁶ to R¹⁸, R³¹ to R³³, R³⁴ to R³⁶, R³⁷ to R³⁹, R⁴⁰ to R⁴² together with the carbon atom to which they are attached each independently form a cyclic alkyl structure.

5

6. A compound as claimed in any one of claims 1 to 3, wherein one or more of the groups R¹ and R², R⁴ and R⁵, R⁷ and R⁸, R¹⁰ and R¹¹, R¹³ and R¹⁴, R¹⁶ and R¹⁷, R³¹ and R³², R³⁴ and R³⁵, R³⁷ and R³⁸, R⁴⁰ and R⁴¹ together with the carbon
10 atom to which they are attached each independently form a cyclic alkyl structure.

7. A compound as claimed in any one of the preceding claims, wherein each of R¹ to R¹⁸ and R³¹ to R⁴² does not
15 represent hydrogen.

8. A compound as claimed in any one of the preceding claims, wherein adamantyl represents unsubstituted adamantyl or adamantyl substituted with one or more
20 unsubstituted C₁-C₈ alkyl substituents, or a combination thereof.

9. A compound as claimed in any one of the preceding claims, wherein 2-phospha-adamantyl represents
25 unsubstituted 2-phospha-adamantyl or 2-phospha-adamantyl substituted with one or more unsubstituted C₁-C₈ alkyl substituents, or a combination thereof.

10. A compound as claimed in any one of the preceding
30 claims, wherein 2-phospha-adamantyl includes one or more oxygen atoms in the 2-phospha-adamantyl skeleton.

11. A compound as claimed in any one of the preceding claims, wherein congressyl represents unsubstituted congressyl.

5 12. A compound as claimed in any one of the preceding claims, wherein R^{50} to R^{53} each independently represent optionally substituted C_1-C_6 alkyl, trifluoromethyl or phenyl optionally substituted with non-substituted C_1-C_6 alkyl or OR^{19} where R^{19} represents non-substituted C_1-C_6
10 alkyl.

13. A compound as claimed in any one of the preceding claims, wherein R^{49} and R^{54} each independently represent hydrogen or non-substituted C_1-C_6 alkyl.

15

14. A compound as claimed in any one of the preceding claims, wherein each of Y^1 to Y^5 represents oxygen.

15. A compound as claimed in any one of the preceding
20 claims, wherein X^1 is identical to X^3 , and X^5 , X^7 and X^9 when present.

16. A compound as claimed in any one of the preceding
25 claims, wherein X^2 is identical to X^4 , and X^6 , X^8 and X^{10} when present.

17. A compound as claimed in any one of claims 1 to 14, wherein X^1 represents $CR^1(R^2)(R^3)$, X^2 represents $CR^4(R^5)(R^6)$, X^3 represents $CR^7(R^8)(R^9)$ and X^4 represents
30 $CR^{10}(R^{11})(R^{12})$.

18. A compound as claimed in any one of claims 1 to 14, wherein X^1 represents $CR^1(R^2)(R^3)$, X^2 represents adamantyl, X^3 represents $CR^7(R^8)(R^9)$ and X^4 represents adamantyl.

5 19. A compound as claimed in any one of claims 1 to 14, wherein X^1 represents $CR^1(R^2)(R^3)$, X^2 represents congressyl, X^3 represents $CR^7(R^8)(R^9)$ and X^4 represents congressyl.

10 20. A compound as claimed in any one of claims 1 to 14, wherein X^1 to X^4 each independently represent adamantyl.

21. A compound as claimed in any one of claims 1 to 14, wherein X^1 to X^4 each independently represent congressyl.

15

22. A compound as claimed in any one of claims 1 to 14, wherein X^1 and X^2 together with Q^2 to which they are attached form a ring system of formula Ia, and X^3 and X^4 together with Q^1 to which they are attached form a ring system of formula Ib.

20

23. A compound as claimed in any one of claims 1 to 14, wherein X^1 and X^2 together with Q^2 to which they are attached form a 2-phospha-adamantyl group, and X^3 and X^4 together with Q^1 to which they are attached form a 2-phospha-adamantyl group.

25

24. A compound as claimed in any one of the preceding claims, wherein K represents hydrogen.

30

25. A compound as claimed in any one of claims 1 to 23, wherein K represents $-A_3-Q^3(X^5)X^6$.

26. A compound as claimed in claim 25, wherein $-A_3-Q^3(X^5)X^6$ is identical to $-A_2-Q^1(X^3)X^4$.

27. A compound as claimed in any one of the preceding
5 claims, wherein D and E together with the carbon atoms of the cyclopentadienyl ring to which they are attached form an unsubstituted phenyl ring.

28. A compound as claimed in any one of the preceding
10 claims, wherein D and E both represent hydrogen.

29. A compound as claimed in any one of claims 1 to 26, wherein D represents $-A_4-Q^4(X^7)X^8$.

15 30. A compound as claimed in claim 29, wherein $-A_4-Q^4(X^7)X^8$ is identical to $-A_2-Q^1(X^3)X^4$.

31. A compound as claimed in any one claims 29 or 30, wherein E represents hydrogen.

20

32. A compound as claimed in any one claims 1 to 26, 29 or 30, wherein E represents $-A_5-Q^5(X^9)X^{10}$.

33. A compound as claimed in claim 32, wherein $-A_5-Q^5(X^9)X^{10}$
25 is identical to $-A_2-Q^1(X^3)X^4$.

34. A compound as claimed in any one of the preceding claims, wherein A_1 and A_2 , and A_3 , A_4 and A_5 when present, each independently represent $-CH_2-$ or $-C_2H_4-$.

30

35. A compound as claimed in any one of the preceding claims, wherein each A_1 and A_2 , and A_3 , A_4 and A_5 when present are identical and preferably represent $-CH_2-$.

36. A compound as claimed in any one of the preceding claims, wherein each Q^1 and Q^2 , and Q^3 , Q^4 and Q^5 when present are identical and preferably represent
5 phosphorous.

37. A compound as claimed in any one of the preceding claims, wherein $n=1$, $m=0$ and L_1 is selected from cyclopentadienyl, phenyl, indenyl or naphthyl, preferably
10 unsubstituted cyclopentadienyl.

38. A compound as claimed in any one of the preceding claims, wherein M represents iron or a metal cation thereof.

15

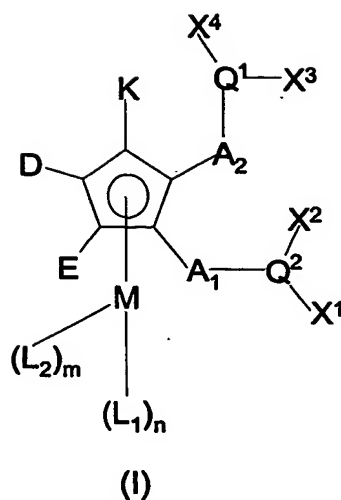
39. A compound as claimed in any one of the preceding claims obtainable by combining: (a) palladium or a compound thereof; and (b) a compound of formula I as defined in any one of the preceding claims.

20

40. A process for preparing a compound as defined in any one of claims 1 to 39 comprising combining (a) a Group VIIIB metal or compound thereof; and, (b) a compound of formula I as defined in any one of claims 1 to 38.

25

41. A compound of formula I

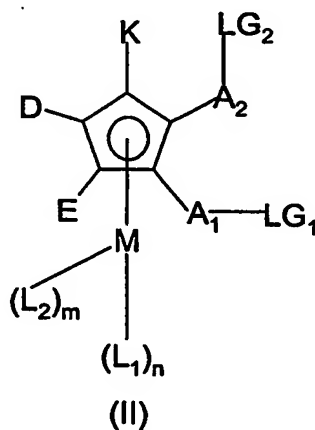


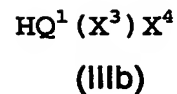
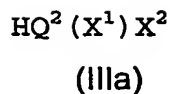
wherein A_1 , A_2 , K , D , E , M , L_2 , L_1 , Q^1 , Q^2 , X^1 , X^2 , X^3 , X^4 , n and m are as defined in any one of claims 1 to 38.

5

42. A process for preparing a compound of formula I as defined in claim 41, comprising reacting a compound of formula II wherein A_1 , A_2 , K , D , E , M , L_1 , L_2 , n and m are as defined for a compound of formula I, and LG_1 and LG_2 represent suitable leaving groups, with a compound of formula IIIa and IIIb

10

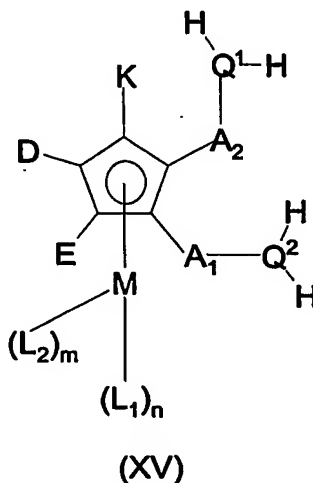




5 wherein X^1 , X^2 , Q^2 , X^3 , X^4 and Q^1 are as defined in anyone of claims 1 to 38.

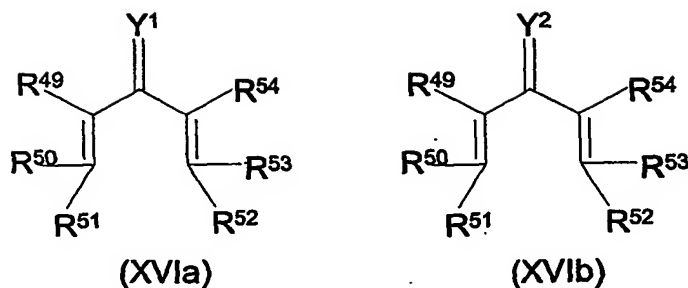
43. A compound of formula II as defined in claim 42.

10 44. A process for preparing a compound of formula I wherein K, D, E, M, A_2 , A_1 , L_2 , L_1 , Q^1 , Q^2 , m and n are as defined in any one of claims 1 to 38 and X^1 and X^2 together with Q^2 to which they are attached form a ring system of formula Ia as defined in anyone of claims 1 to
 15 38 and X^3 and X^4 together with Q^1 to which they are attached form a ring system of formula Ib as defined in any one of claims 1 to 38, comprising reacting a compound of formula XV



20

wherein K, D, E, M, A_2 , A_1 , L_2 , L_1 , Q^1 , Q^2 , m and n are as defined in any one of claims 1 to 38, with a compound of formula XVIa and XVIb



wherein Y¹, Y², R⁴⁹ to R⁵⁵ are as defined for a compound of formula I.

5

45. A compound of formula XV as defined in claim 44.

46. A process for the carbonylation of an ethylenically unsaturated compound comprising contacting an
 10 ethylenically unsaturated compound with carbon monoxide and a co-reactant in the presence of a compound as defined in any one of claims 1 to 39.

47. A process as defined in claim 46 wherein the co-
 15 reactant includes a hydroxyl group containing compound.

48. A process as claimed in claim 46 or 47 wherein the ethylenically unsaturated compound comprises ethylene, 1,3-butadiene, oct-1-ene or vinyl acetate, preferably
 20 ethylene.

49. A process as claimed in any one of claims 46 to 48, further including the step of including a source of anions.

25

50. A composition comprising a compound as defined in any one of claims 1 to 39 attached to a support.

51. Use of a compound as defined in anyone of claims 1 to 39 or a composition as defined in claim 50 as a catalyst.